Higher Order Perturbation Theory

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The Interaction Representation

Recall that in the first part of this course sequence, we discussed the Schrödinger and Heisenberg representations of quantum mechanics here. In the Schrödinger representation, the operators are time-independent (except for explicitly time-dependent potentials) the kets representing the quantum states develop in time. In the Heisenberg representation, the kets stay the same, the time dependence is in the operators. These differing representations describe the same physics—matrix elements of operators between kets must be the same in both. The most natural to use depends on the problem at hand. In the classical limit, for example, the Heisenberg operators have the time dependence of the corresponding classical operators.

In fact, for perturbation theory problems with a time-dependent potential, an intermediate representation, the *interaction representation*, is very convenient. Using a subscript S to denote the Schrödinger representation,

$$i\hbar\frac{d}{dt}\left|\psi_S(t)\right\rangle = H_S\left|\psi_S(t)\right\rangle = \left(H_S{}^0 + V_S(t)\right)\left|\psi_S(t)\right\rangle,$$

we define the *interaction representation* by the unitary transformation

$$\left|\psi_I(t)\right\rangle = e^{iH_S^0 t/\hbar}\left|\psi_S(t)\right\rangle$$

so the interaction representation kets and the Schrödinger representation kets coincide at $t = 0$, and if the interaction were zero, the interaction representation kets would be constant in time, like those in the Heisenberg representation.

For nonzero $V(t)$, then, the time development of the interaction representation kets is entirely due to $V(t)$, and is easily found by differentiating both sides of the equation:

$$\begin{aligned}
i\hbar\frac{d}{dt}\left|\psi_I(t)\right\rangle &= -H^0\left|\psi_I(t)\right\rangle + e^{iH_S^0 t/\hbar} i\hbar\frac{d}{dt}\left|\psi_S(t)\right\rangle \\
&= -H^0\left|\psi_I(t)\right\rangle + e^{iH_S^0 t/\hbar}\left(H_S^0 + V_S(t)\right)e^{-iH_S^0 t/\hbar}\left|\psi_I(t)\right\rangle \\
&= e^{iH_S^0 t/\hbar}V_S(t)e^{-iH_S^0 t/\hbar}\left|\psi_I(t)\right\rangle \\
&= V_I(t)\left|\psi_I(t)\right\rangle,
\end{aligned}$$

where we have introduced the interaction representation operator $V_I(t)$, defined by

$$V_I(t) = e^{iH_S^0 t/\hbar}V_S(t)e^{-iH_S^0 t/\hbar}.$$

Operators in this representation must have this time dependence relative to the Schrödinger operators to ensure that matrix elements, the only quantities of physical significance, are the same in the two representations. That is to say, we must have

$$\left\langle f_I^0 \middle| O_I \middle| i_I^0 \right\rangle = \left\langle f_S^0 \middle| O_S \middle| i_S^0 \right\rangle,$$

the two representations must predict the same probability amplitude for any transition.

Integrating both sides of the differential equation,

$$\left|\psi_I(t)\right\rangle = \left|\psi_I(0)\right\rangle - \frac{i}{\hbar}\int_0^t dt' V_I(t')\left|\psi_I(t')\right\rangle.$$

This is not a solution—we've just gone from a differential equation to an integral equation. This is only worth doing if V_I is small, in which case the integral equation can be solved iteratively.

The zeroth approximation is then

$$\left|\psi_I(t)\right\rangle = \left|\psi_I(0)\right\rangle.$$

Putting this value into the small term on the right hand side of the integral equation gives the first order solution,

$$\left|\psi_I(t)\right\rangle = \left|\psi_I(t_0)\right\rangle - \frac{i}{\hbar}\int_0^t dt' V_I(t')\left|\psi_I(0)\right\rangle.$$

The second order solution is now given by putting the first order solution into the integral on the right:

$$\left|\psi_I(t)\right\rangle = \left|\psi_I(0)\right\rangle - \frac{i}{\hbar}\int_0^t dt' V_I(t')\left(\left|\psi_I(0)\right\rangle - \frac{i}{\hbar}\int_0^{t'} dt'' V_I(t'')\left|\psi_I(0)\right\rangle\right).$$

This can be written:

$$\left|\psi_I(t)\right\rangle = \left(1 - \frac{i}{\hbar}\int_0^t dt' V_I(t') + \left(-\frac{i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' V_I(t') V_I(t'')\right)\left|\psi_I(0)\right\rangle.$$

The complete perturbation series is generated by repeating the iteration to all orders. It can be expressed as a *time-ordered product*:

$$\left|\psi_I(t)\right\rangle = T\exp\left(-\frac{i}{\hbar}\int_0^t dt' V_I(t')\right)\left|\psi_I(0)\right\rangle .$$

The T symbol means that on expanding out the exponential, the operators at different times are arranged in order of time, the latest on the left, without worrying about commutators. If we just blindly expand the exponential, we will get, for example, a third-order term

$$T\frac{1}{3!}\left(-\frac{i}{\hbar}\int_0^t dt' V_I(t')\right)\left(-\frac{i}{\hbar}\int_0^t dt'' V_I(t'')\right)\left(-\frac{i}{\hbar}\int_0^t dt''' V_I(t''')\right).$$

The T operator tells us to rearrange the $V_I(t)$'s in chronological order. Since there are three of them, they clearly appear in all possible orders before T operates, that is to say, there are 3! different ordered terms that T makes the same. This just nicely cancels the 3! in the exponential expansion, to give us the expression we found by iteration.

This time-ordered exponential is therefore the *interaction representation propagator*:

$$\left|\psi_I(t)\right\rangle = U_I(t,0)\left|\psi_I(0)\right\rangle, \quad U_I(t,0) = T\exp\left(-\frac{i}{\hbar}\int_0^t dt' V_I(t')\right).$$

Going Back to the Schrödinger Representation

It is instructive to recast this result in the Schrödinger representation (following Shankar). First, note that putting the above equation for U_I together with the original definition of interaction representation kets

$$\left|\psi_I(t)\right\rangle = e^{iH_S^0 t/\hbar}\left|\psi_S(t)\right\rangle$$

gives

$$\left|\psi_S(t)\right\rangle = e^{-iH_S^0 t/\hbar}\left|\psi_I(t)\right\rangle = e^{-iH_S^0 t/\hbar}U_I(t,0)\left|\psi_I(0)\right\rangle = e^{-iH_S^0 t/\hbar}U_I(t,0)\left|\psi_S(0)\right\rangle .$$

So the Schrödinger representation propagator is related to the interaction representation propagator by:

$$U_S(t,0) = e^{-iH_S^0 t/\hbar}U_I(t,0).$$

Now let us see how to put our perturbation expansion for the propagator back from the interaction representation into the Schrödinger representation. Instead of trying to handle the whole infinite series at once, we concentrate on the second-order term. We will discover a pattern that works for all the higher order terms as well.

So, transforming the operators in the second-order term of the interaction propagator back to the Schrödinger form, using

$$V_I(t) = e^{iH_S^0 t/\hbar} V_S(t) e^{-iH_S^0 t/\hbar}$$

we find

$$\left(\frac{1}{i\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' V_I(t') V_I(t'') = \left(\frac{1}{i\hbar}\right)^2 \int_0^t \int_0^{t'} dt' dt'' e^{iH_S^0 t'/\hbar} V_S(t') e^{-iH_S^0 t'/\hbar} e^{iH_S^0 t''/\hbar} V_S(t'') e^{-iH_S^0 t''/\hbar}.$$

Recall also that the Schrödinger propagator has the extra term $e^{-iH_S^0 t/\hbar}$ multiplying the interaction representation propagator. Putting this in, and combining some of the exponentials, we find the second-order contribution to the Schrödinger propagator to be:

$$\left(\frac{1}{i\hbar}\right)^2 \int_0^t \int_0^{t'} dt' dt'' e^{-iH_S^0 (t-t')/\hbar} V_S(t') e^{-iH_S^0 (t'-t'')/\hbar} V_S(t'') e^{-iH_S^0 t''/\hbar}$$

which can also be written:

$$\left(\frac{1}{i\hbar}\right)^2 \int_0^t \int_0^{t'} dt' dt'' U_S^0(t,t') V_S(t') U_S^0(t',t'') V_S(t'') U_S^0(t'',0).$$

To find the probability amplitude corresponding to this second-order process, we must sandwich it between initial and final states. We take as our basis set the eigenstates of $H_S{}^0$. If we insert the unit operator

$$I = \sum_n \left|n^0\right\rangle\left\langle n^0\right|$$

between the two V_S's, the exponentiated $H_S{}^0$'s become simply numbers since they are now acting on eigenstates, and the expression becomes

$$\left(\frac{1}{i\hbar}\right)^2 \int_0^t \int_0^{t'} dt' dt'' e^{-iE_f^0 (t-t')/\hbar} \left\langle f^0\right| V_S(t') \left|n^0\right\rangle e^{-iE_n^0 (t'-t'')/\hbar} \left\langle n^0\right| V_S(t'') \left|i^0\right\rangle e^{-iE_i^0 t''/\hbar}.$$

The interpretation is now clear: the initial state $\left|i^0\right\rangle$ evolves from $t = 0$ to t'' under $H_S{}^0$, that is to say, only its phase changes in the standard fashion. At t'', the interaction $V_S(t'')$ kicks it into another eigenstate $\left|n^0\right\rangle$ of $H_S{}^0$, and only the phase changes until t', when $V_S(t')$ sends it to the final state $\left|f\right\rangle$. This process must be summed over all times t', t'' between t_0 and t, and over all possible intermediate states.

The n^{th} order term has precisely the same structure, with V_S coming into play n times.